Ion beam analysis of Fe-based Heusler alloys/Ge hetero-epitaxial interfaces toward spin transistors

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Our Research

Silicide Science and Technology
Ion Beam Synthesis of iron silicides

Iron silicide nanostructures for light emitter

Iron silicide photonic crystals

Ion Beam Analysis of ferromagnetic silicide/semiconductor hybrid structure
Prof. M. Miyao, Prof. K. Hamaya, Prof. T. Sadoh
Kyushu University,
on MBE of ferromagnetic alloy films on semiconductors

Dr. M. Narumi, Dr. S. Sakai, Dr. K. Takahashi
Japan Atomic Energy Agency (JAEA)
on Ion beam analysis and development of beam lines
toward low temperature ion channeling experiments

Students graduated from Maeda Laboratory,
at Kyoto University, on RBS measurements.

Prof. Y. Terai, Dr. Y. Ando, Osaka University
on characterization of films
1. Motivation
   Ion Beam Analysis of materials for Spintronics.
2. Ion Channeling and its application to
   quantitative evaluation of disordering of some Heusler alloy films epitaxially grown on Ge(111).
3. Topic : Spin injection behavior related to quality of epitaxial growth of ferromagnetic (FM) Heusler alloy films Fe$_3$Si on Si(111).
4. Conclusions
One of Goals of Spintronics, Spin FET

Spin-FET has a same device structure as MOSFET. We expect it on very high frequency operation and very low consuming power.

FM source epitaxially grown on Ge(111)

High quality heteroepitaxial interface realized by low temperature MBE technique.

Efficiency of Spin Injection from FM into SC

$$\alpha = \frac{P_{SC}}{P_{FM}}$$

$$= \frac{1}{1 + (1 - P_{FM})^2 \left( \frac{R_{SC}}{R_{FM}} \right)^2}$$

$P_{FM}$: Spin polarity of FM
$R_{sc}$: Electrical resistivity of SC
$R_{F}$: Electrical resistivity of FM

In usual case, $R_{sc} >> R_{F}$, so that $\alpha << 1$

that is, Resistivity gap problem,
we have to overcome it for Spintronics.
Possible solutions

- Using *half metallic FM material* as an electrodes such as Fe$_2$MnSi etc. (if possible, the problem remains.)
- Using Magnetic SC with highly polarized spin states. (in future, possible?)
- Using spin injection by *electron tunneling through a Schottky barrier*. (Actually promising)

K. Takanashi, JJAP (2011)
Spin injection by electron tunneling through Schottky barrier

FM metal → n-type SC

Conditions for Spin injection

*We need* thinner barrier width enough to cause electron tunneling and higher barrier height enough to prevent thermal emission.

- Delta dope technology
- Reduction of interface states by high quality MBE
**Fe\(_{3-x}\)Mn\(_x\)Si (FMS) : Spin polarization**

L\(_2\)\(_1\) type Heusler alloy with ordered lattice Fe\(_2\)MnSi

Stoichiometric Fe\(_2\)MnSi is estimated to be half metallic. Mn occupation at the B site affects spin polarization as shown in right figure.

Low temperature MBE realized High quality Epitaxy

Low Temperature MBE

Growth Temp. <200°C

<table>
<thead>
<tr>
<th>Layer</th>
<th>Fe</th>
<th>Si</th>
<th>Mn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ge(111)</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Ge buffer layer</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Fe₃Si or Fe₂MnSi</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Fe₂CoSi</td>
<td></td>
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</tbody>
</table>

Fe Si Mn
Fe₃Si 0.12 0.04
Fe₂MnSi 0.047 0.04 0.015

Co-evaporation

RHEED Patterns

Ge buffer
Fe₃Si
Fe₂MnSi

B//<211>

Growth temperature $T_G$ is crucial for high quality epitaxy of FM $F_3Si/Ge$

Low $T_G$ is much better, we can prevent active interdiffusion between FM and Ge substrates and keep a DO$_3$ ordered lattice during growth.
XTEM, SAD observations of $\text{Fe}_2\text{MnSi}(111)/\text{Ge}(111)$


XTEM brings direct information of epitaxial interfaces, however, does not teach the in-plane information at spin injection interfaces to us.
2. Introduction to Ion Channeling and its application to Quantitative analysis of disordering of some Heusler alloy films epitaxially grown on Ge(111).
Ion Beam Analysis involves the use of an energetic ion beam to probe the surface of a material to reveal details of the elemental and structural details of it make up.

* cited from SCRIBA, University of Surrey
Why do we need IBA?

IBA: Ion Beam Analysis

Using IBA, we can obtain not only atomic information at a tentative spin injection interface but also information from surface and the interface under nondestructive sample conditions.
Advantages of IBA

- Nondestructive under low dose of incident ions
- Element resolution analysis
- Depth analysis
- Average information at analyzing macro-area
- Usage of channeling techniques for analysis of depth distribution of disorder, location of impurity
Rutherford Backscattering

- **Random scattering** gives information of depth distribution of elements involved in a sample.

  Projection of atomic raw tilted by 5 degrees seems a random atomic arrangement.

- **Channeling** gives information of amount and depth distribution of disorder, location of impurity in the lattice site, and composition and thickness of disordered surface layer.

  &lt; Ge<111> raw

*Wei-Kan Chu et al., Backscattering Spectrometry, AP*
incident Ions from a specific direction into crystals can travel inside of the crystal channel, so that backscattering yield and stopping power decreases drastically.
Alignment of crystal axis, Case of Ge\(<111>\)

On Ge(111) plain, the zone axis of Ge\(<111>\) can be found by tilting along two specific direction, X and Y. This alignment of the axis controls accuracy of ion beam channeling.
RBS measurements at JAEA-TIARA

Dual Beam Analysis Line (MD2)
ion channeling set-up at low temperature

(Cited from Homepage of JAEA-TIARA)
Rutherford Backscattering (RBS)

Random scattering spectrum (Random RBS)

\[ \text{SIMNRA}^{\text{Ⓡ}} \text{fitting} \]

\[ \theta > 4 \text{ deg.} \]

\[ 2\text{MeV}^{-4}\text{He}^+ \]

\[ \text{Si}_3-x\text{Mn}_x\text{Si} \ x = 0.84 \]

Ge substrate

Fe channel

Mn channel

Si channel
When a sample is tilted from aligned angle, RBS spectrum changes continuously from channeling to random scattering.
Angular yield profiles, Channeling parameter

\[ \chi(\theta) = 1 - (1 - \chi_{\text{min}}) \exp \left( -\ln 2 \left( \frac{\theta - \theta_0}{\psi_{1/2}} \right)^m \right) \]

Using the upper equation, deconvolution of angular yield profile for Fe and Mn can be performed and channeling parameter \( \chi_{\text{min}} \) and \( \psi_{1/2} \) were obtained.
Fe$_{3-x}$Mn$_x$Si/Ge(111) hybrid structure at interfaces

We observed systematic increase of the minimum yield and decrease of the critical half angle as Mn content increased. All FMS with each Mn content maintained epitaxy with Ge(111).

Angular yield profiles at the interfaces with Ge(111)

**FMS/Ge**

Fe$_2$MnSi/Ge(111)

\[ \chi_{\text{min}} = 0.045 \]

\[ \psi_{1/2} = 0.85 \text{deg.} \]

**300K**

**FCS/Ge**

Fe$_2$CoSi/Ge(111)

\[ \chi_{\text{min}} = 0.013 \]

\[ \psi_{1/2} = 0.88 \text{deg.} \]
Summary of results

Minimum yield $\chi_{\text{min}}$

Half angle $\psi_{1/2}$ (degree)

Perfect crystal line with Debye temperature $\Theta_D = 420$ K

FS

FCS

FMS

21 at% Mn

18 at% Mn

9 at% Mn

Fe$_3$Si

Fe$_2$CoSi

worse

better

worse

better
Toward quantitative analysis using channeling parameter

Barrett-Gemmell model teaches us the way to quantitative analysis using channeling parameter ($\chi_{\text{min}}$, $\psi_{1/2}$).

$$\chi_{\text{min}} = 18.8Nd\langle u \rangle^2 \sqrt{1 + \frac{1}{\zeta^2}}$$

$$\zeta = \frac{126\langle u \rangle}{\psi_{1/2}d}$$

$\langle u \rangle$: total atomic displacement
N: atomic density
d: interatomic spacing in axial directions

Fortunately, we can solve above simultaneous equations using elementary mathematics.

How can we deduce \( <u> \) from channeling parameter?

\[
\begin{align*}
(\chi_{\text{min}}, \psi_{1/2}) & \quad \Rightarrow 2 \\
A &= \left( \frac{\psi_{1/2}d}{126} \right)^2, \quad B = \left( \frac{\chi_{\text{min}}}{18.8Nd} \right)^2 \\
\langle u \rangle(\text{A}) &= \frac{1}{\sqrt{2}} \sqrt{\sqrt{A^2 + 4B} - A}
\end{align*}
\]

Remarks: under the condition at the same energy of incident ions


Total atomic displacement along atomic row

Total displacement can be written by sum of contributions of thermal vibration and static displacement due to some imperfection in the atomic row.

\[
\langle u \rangle^2 = \langle u_{th} \rangle^2 + \langle u_s \rangle^2
\]

For perfect crystals or crystals with small imperfection being not detectable

\[
\langle u \rangle^2 = \langle u_{th} \rangle^2
\]
Calculation of $<u_{th}>$

Debye model teaches us the one dimensional thermal vibration of a given atom, if the Debye temperature $\Theta_D$ of material is known.

Only for $i$-th element,

$$
\langle u_{th} \rangle (\text{Å}) = 12.1 \left[ \left( \frac{\phi(y)}{y} + \frac{1}{4} \right) / \mu_i \Theta_D \right]^{1/2}
$$

$$
\phi(y) = \frac{1}{y} \int_0^y \frac{t}{e^t - 1} dt, \quad y = \frac{\Theta_D}{T} \quad \mu_i : \text{reduced mass}
$$

Wei-Kan Chu et al.,
Backscattering Spectrometry, AP
First order Debye function

\[ \phi(y) = \frac{1}{y} \int_0^y \frac{t}{e^t - 1} \, dt, \]

\[ y = \frac{\Theta_D}{T} \]

Case of Fe$_2$MnSi

\( \Theta_D = 420\text{K} \)
\( T = 300\text{K} \)
\( y = 1.4 \)
Calculation of static displacement $<u_s>$ due to imperfection

\[(i) \quad \langle u \rangle^2 \geq \langle u_{th} \rangle^2 \]

\[\langle u_s \rangle = \sqrt{\langle u \rangle^2 - \langle u_{th} \rangle^2} \]

\[(ii) \quad \langle u \rangle^2 \leq \langle u_{th} \rangle^2 \]

\[\langle u_s \rangle = 0 \quad \text{corresponding to perfect crystals or crystals with not detectable imperfection} \]

The static displacement can be obtained from subtraction between measured total displacement and calculated thermal vibration.
Static atomic displacement $<u_s>$ at interface

Lattice mismatch between FMS and Ge

$$\delta(x) = \left( \frac{(5.653 + 0.011x) - 5.657}{5.657} \right) \times 100$$

Fe$_{3-x}$Mn$_x$Si

Ge(111)

Zero mismatch

at 300 K

Fe$_3$Si/Ge

Strong correlation between $<u_s>$ and lattice mismatch $\delta$ at the interface was found. This means that imperfection may mainly be introduced by the lattice mismatch.

This difference may come from B site randomness due to Mn occupation.
These FMR measurements give the first confirmation that crystal quality of Fe$_3$Si directly controls performance of spin injection.
Conclusions

• Ion beam analysis (IBA) is helpful and powerful for analysis of epitaxial hetero-interfaces.
• It is possible to deduce quantitative and average information such as atomic displacements at a given depth or interface from the ion channeling parameter.
• Most recently, spin injection experiments are going more active. IBA data will be helpful for understanding its properties.
Thank you for your kind attention!
Ion channeling of Fe$_3$Si, Fe$_4$Si/Si(111)

LTMBE

Results of ion channeling and static atomic displacement and spin injection experiment

<table>
<thead>
<tr>
<th></th>
<th>$\delta$(%) at IF</th>
<th>$\chi_{\text{min}}$</th>
<th>$\psi_{1/2}$(deg.)</th>
<th>$&lt;u_s&gt;$(A)</th>
<th>emf (mV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe$_3$Si/Si</td>
<td>+4.13</td>
<td>0.18</td>
<td>0.99</td>
<td>0.25</td>
<td>~68</td>
</tr>
<tr>
<td>Fe$_4$Si/Si</td>
<td>+4.15</td>
<td>0.23</td>
<td>0.95</td>
<td>0.52</td>
<td>~18</td>
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<tr>
<td>Fe$_3$Si/Ge</td>
<td>-0.05</td>
<td>0.02</td>
<td>0.98</td>
<td>0.09</td>
<td></td>
</tr>
</tbody>
</table>
Dynamical spin injection into Pd layer using Fe₃Si

High quality Single crystalline Fe₃Si

① Large EMF

Fe₃Si

Py

② Control experiments

Only Fe₃Si

Al / Fe₃Si

To realize highly efficient generation of pure spin current...
✓ High quality FM layer with uniform magnetic properties.
✓ Small Gilbert damping constant
⇒ Ferromagnetic silicide Fe₃Si with homogeneous quality is promising.

(Y. Andoh, APEC-SILICIDE 2013)
Comparison of EMF for various FM samples

\[ V_{\text{ISHE}}/w = 67.1 \ \mu\text{V/mm} \]

\[ V_{\text{ISHE}}/w = 3.05 \ \mu\text{V/mm} \]

\[ V_{\text{ISHE}}/w = 2.92 \ \mu\text{V/mm} \]

(Y. Andoh, APEC-SILICIDE 2013)
Fe$_2$MnSi(111)/Ge(111) $T_d=200^\circ$C

Intermixing layer
We found that increase of Mn content at the B site brings randomness of the atomic row along <111> direction. This behavior has been observed as increase of a Debye-Waller factor in EXAF, XANES measurements. Randomness along <111> may be introduced by weak chemical bonds around Mn atoms at the B site.